Electronic supplementary information

Ligand synthesis

The procedure for the synthesis of ligand L is depicted in Scheme S1. 2,9-bis(bromomethyl)-1,10-phenanthroline **E** was prepared as previously described. (Chandler, C.J.; Deady L.W., Reiss J. A.. J. Heterocycl. Chem. 1981, 18, 599.)

1,21-Phthalimido-5,9,13,17-tetrakis(*p*-tolylsulfonyl)-1,5,9,13,17,21-hexaazahenicosane (B)

Tosylated amine 1,4,8,12-tetratisyl-1,4,8,12-tetrazadodecane **A** (10.06 g, 12.5 mmol), K_2CO_3 (13.82 g, 0.1 mol) and *N*-(3-bromopropyl)phthalimide (13.40 g, 50 mmol) were suspended in refluxing CH_3CN (300 cm^3). After refluxing for 12 h, the suspension was filtered off. The solution was vacuum evaporated to dryness and the crude product was chromatographated on neutral alumina ligroin-ethyl acetate 1:1 mixture. The eluted fractions were collected and evaporated to dryness to afford **B** as yellowish oil. Yield: 14.44 g, 98%; Anal. Calcd. for $C_{59}H_{66}N_6S_4O_{12}$: C, 60.1; H, 5.64; N, 7.13. Found C, 60.2; H, 5.7; N, 7.2. ^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.82 (m, 4H), 7.66 (m, 12H), 7.28 (t, 8H), 3.68 (t, 4H), 3.13 (m, 16H), 2.42 (s, 6H), 2.40 (s, 6H), 1.89 (m, 10H). ^{13}C-NMR ($CDCl_3$, 75 MHz) δ 167.9, 143.2 , 135.9, 133.8, 134.0, 131.8, 129.6, 129.4, 127.0, 127.3 , 123.0, 122.8, 46.3, 46.6, 46.8, 46.2, 46.5, 46.7 , 35.5, 35.2, 34.9, 27.7, 27.5, 27.2, 21.4,21.2, 20.9, 20.7.

5,9,13,17-Tetrakis(*p*-tolylsulfonyl)-1,5,9,13,17,21-hexaazahenicosane (C)

A mixture of compound **B** (14.44 g, 12.2 mmol) and hydrazine monohydrate 85% (30 mL, 0.69 mol) in THF (500 mL) was refluxed for 12 h. Then the mixture was cooled, filtered off and the solution was vacuum evaporated to dryness to give a yellowish oil . The oil was dissolved in 100 mL of $CHCl_3$ and the solution was dried with anhydrous Na_2SO_4. Then, it was vacuum evaporated to dryness to obtain product **C**. Yield: 11.1 g, 99%. Anal. Calcd for $C_{43}H_{62}N_6S_4O_8$ C, 55.77; H, 6.08; N, 6.85. Found C, 55.8; H, 6.1; N, 6.9. ^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.66 (d, 8H), 7.30 (m, 8H), 3.14 (m, 16H), 2.70 (t, 4H), 2.42 (s, 12H), 1.90 (m, 6H), 1.64 (m, 4H).

1,5,9,13,17,21-Hexakis(*p*-tolylsulfonyl)-1,5,9,13,17,21-hexaazahenicosane (D)

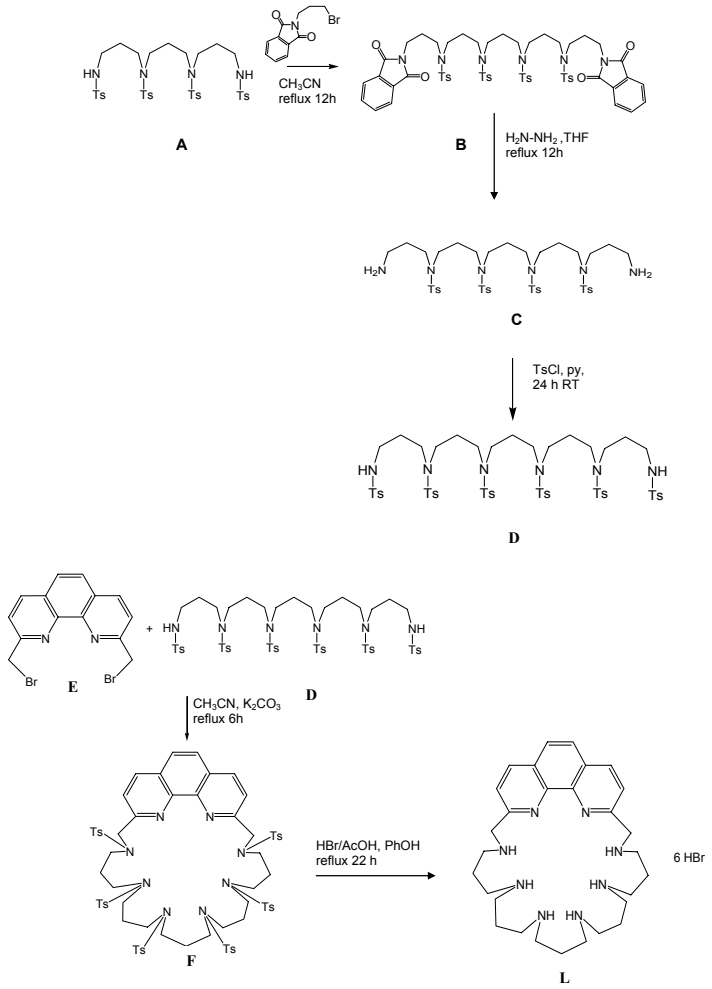
A solution of **C** (10.91g, 12 mmol) in 50 mL of pyridine was added in four hours under vigorous stirring to a solution of *p*-tolylsulfonyl chloride (6.62 g, 35 mmol) dissolved in 50 ml of pyridine; the reaction temperature was kept at 10 °C. The reaction mixture was then kept under stirring at room temperature overnight. The solution was then added to a vigorously stirred mixture of water and ice. The product obtained was filtered off, washed with water and ethanol, recrystallized from a chloroform-ethanol mixture and dried in vacuo at 40 °C. Yield: 12.1 g (82%). Anal. Calcd for $C_{57}H_{74}N_6S_6O_{12}$ C, 55.77; H, 6.08; N, 6.85. Found C, 55.8; H, 6.1; N, 6.9 ^{1}H-NMR ($CDCl_3$, 300 MHz) δ 7.68 (m, 12H), 7.30 (m, 12H), 3.13 (m, 16H), 2.98 (t, 4H), 2.42 (m, 18H), 1.85 (m, 10H,). ^{13}C-NMR ($CDCl_3$, 75 MHz) δ 143.5, 136.8, 129.8, 129.6, 127.1, 127.0, 47.5, 47.0, 46.7, 40.2, 40.3, 40.5, 29.4. 29.2, 29.0, 21.5, 21.2, 21.0, 19.8.

2,6,10,14,18,22-hexa(*p*-tolylsulfonyl)-2,6,10,14,18,22-hexaaza [23]-24,37-phenanthrolinophane. (F)

A sample of **D** (8.0 g, 6.5 mmol) and K_2CO_3 (9.02 g, 65 mmol) were suspended in refluxing CH_3CN (300 mL). To this mixture, a solution of 2,9-bis(bromomethyl)-1,10-phenanthroline **E** (2.38 g, 6.5 mmol) in CH_3CN (500 mL) was added dropwise in 4 h. After the addition was completed, the suspension was refluxed for 2 h and then filtered. The solution was vacuum evaporated to yield the crude product which was chromatographated on neutral alumina by using ligroin-ethyl acetate 1:1.5 as eluent. The eluted fractions were collected and evaporated to dryness to afford compound **F** as a colorless solid (2.78 g, 30%). Anal. Calcd for $C_{71}H_{82}N_8S_6O_{12}$ C, 59.56; H, 5.77; N, 7.83. Found C, 59.4; H, 5.9; N, 7.8. ^{1}H-NMR ($CDCl_3$, 300 MHz) δ 8.30 (d,2H), 7.96 (d, 2H), 7.80 (s, 2H), 7.71 (d, 4H), 7.53 (m, 8H), 7.26 (m, 12H), 4.76 (s, 4H), 3.25 (t, 4H), 2.97 (t,4H), 2.76 (m, 12H), 2.38 (s, 18H), 1.64 (m, 6H), 1.30 (m, 4H). ^{13}C-NMR ($CDCl_3$, 75 MHz) δ 157.9, 143.4, 143.2, 143.1, 137.2, 135.6, 135.6, 129.7, 129.6, 128.0, 127.1, 127.0, 77.2, 55.6, 48.0, 46.9, 46.6, 46.4, 46.2, 28.5, 28.3, 28.2, 21.5.

2,6,10,14,18,22-hexaaza [23]-24,37-phenanthrolinophane Hexahydrobromide (L· 6HBr).

Hexatosylated macrocycle **F** (2.78 g, 1.94 mmol) and phenol (32.70 g, 0.35 mol) were dissolved in HBr/AcOH (33%, 270 mL). The solution was stirred at 90 °C for 22 h. The resulting suspension was filtered, and the solid was washed with CH_2Cl_2 for several times. The yellowish solid was recrystallized from a water/ethanol mixture to give **L** as hexahydrobromide salt (1.31 g, 68%). Anal. Calcd for $C_{29}H_{52}N_8Br_6$ C, 35.11; H, 5.28; N, 11.29. Found C, 35.1; H, 5.2; N, 11.2. ^{1}H-NMR (D_2O, 300 MHz) δ 8.50 (d, 2H), 7.92 (s, 2H), 7.84 (d, 2H), 4.72 (s, 4H), 3.50 (t, 4H), 3.36-3.27 (m, 16H), 2.40-2.32 (m, 4H), 2.27-2.20 (m, 6H). ^{13}C-NMR (D_2O, 75 MHz) δ 151.1, 144.2, 139.2, 129.1, 127.3, 123.3, 52.3, 45.2, 44.8, 44.7, 44.1, 44.0, 23.0, 22.5, 21.8. MS (ESI) m/z 507.42 (100) $(M+H)^+$, 254.21 (68) $(M+2H)^{2+}$.



Scheme S1

Potentiometric measurements. The protonation constants of L and the formation constants of its anion complexes were determined by means of potentiometric measurements (pH = -log $[H^+]$) carried out in 0.1 mol dm^{-3} NMe_4Cl at 298.1 ± 0.1 K in the pH range 2.5-11. The reference electrode was an Ag/AgCl electrode in saturated KCl solution. The glass electrode was calibrated as a hydrogen concentration probe by titrating known amounts of HCl with CO_2-free NaOH solutions and determining the equivalent point by the Gran's method (G. Gran, *Analyst* (London), 1952, **77**, 661. F. J. Rossotti and H. Rossotti, *J. Chem. Educ.* 1965, **42**, 375) which allows to determine the standard potential E^o, and the ionic product of water (pK_W = 13.83 ± 0.01). Ligand concentration was about 1.10^{-3} M, while substrate concentration was in the range 5.10^{-3}-5.10^{-4} M. At least three measurements (about 100 experimental points each one) were performed for each system. The computer program HYPERQUAD (P. Gans, A. Sabatini and A. Vacca, *Talanta*, 1996, **43**, 807) was used to calculate the protonation constants and the stability constants of the complexes from e.m.f. data. The titration curves for each system were treated either as a single set or as separated entities without significant variations in the values of the basicity constants.

Generation of the selectivity plot. The selectivity plot in Figure 2 was obtained from the equilibrium constants given in Table S1 and S2 by using the computer program HYSS 2.0 (L. Alderighi, P. Gans, A. Ienco, D. Peters, A. Sabatini and A. Vacca, *Coord. Chem. Revs.,* **1999***,* 184, 311-318; the program can be downloaded free of charge at http://www.chim1.unifi.it/group/vacsab/hyss.htm). This program takes as input a set of equilibrium constants (in the present case the protonation constants of ligand and nucleotides, Table S1, and the cumulative formation constants of the adducts of ATP, TTP, CTP and GTP, Table S2) and reagent initial concentrations (in the present case [L] = [ATP] = [CTP] = [TTP] = [GTP] = $1x10^{-4}$ M) and calculates from these data the concentrations of all the

complexed species formed (in the present case the concentrations of the products of the reactions given in Table S2) as a function of pH. For each nucleotide, the calculated concentrations of the complexed species at a given pH are then summed, affording the overall concentration of L complexed species with each nucleotide, i.e., $\Sigma[(H_nLATP)^{(n-4)+}]$, $\Sigma[(H_nLCTP)^{(n-4)+}]$, $\Sigma(H_nLTTP)^{(n-4)+}]$, $\Sigma[(H_nLGTP)^{(n-4)+}]$. These values are then divided by the initial concentrations of the ligand L ($1x10^{-4}$ M in the present case), obtaining the overall percentage of L complexed species with each nucleotide at a given pH value. This calculation is repeated all over the pH range of interest (2-10 in the present case), affording the overall percentage of L complexed species with each nucleotide as a function of pH, reported in Figure 2.

Spectroscopic measurements. ^{1}H, ^{13}C and ^{31}P NMR spectra in D_2O solutions at different pH values were recorded at 298 K in a Varian 300 MHz spectrometer. ^{1}H-^{1}H and ^{1}H-^{13}C 2D correlation experiments were performed to assign the signals. In the NMR titrations small amounts of 0.01 mol dm^{-3} NaOD or DCl solutions were used to adjust the pD. The pH was calculated from the measured pD values using the relationship: pH = pD - 0.40 (A. K. Covington, M. Paabo, R. A. Robinson and R. G. Bates, *Anal. Chem.* 1968**, 40**, 700.) UV-vis and fluorescence emission spectra were recorded respectively on a Perkin-Elmer Lambda 25 and LS-55 spectrometers at 298 K.

MD calculations. MD calculations were performed by using the AMBER3 forcefield, as implemented in the Hyperchem 7.51 package (Hyperchem β1 release 7.51 for Windows MM System, Hypercube, Inc., Gainesville, FL, 32601). Atomic charges for receptors and substrates were calculated at the PM3 semiempirical level. (J. P. P. Stewart, *J. Comput.-aided Mol. Des.,* 1990, **4**, 1) Starting conformations of the $[H_6LATP]^{2+}$ or $[H_6LCTP]^{2+}$ adducts, obtained by manual docking of the minimized conformer of the receptor to the substrate

(minimum distance between the atoms of receptor and substrate > 5 Å), were freely minimized. The Polak-Ribiere (coniugate gradient) algorithm was used in the minimization procedures to a root-mean-square (RMS) energy gradient less than 0.001 kcal mol^{-1} $Å^{-1}$. Potential energy surface of both adducts was explored by means of simulated annealing (running temperature = 600 K, equilibration, running and cooling time = 10 ps, time step = 1.0 fs). For each $[H_6LA]^{2+}$ adduct, 80 conformations were sampled, which were subsequently clusterized (RMS ≤ 1.0 Å). A distance-dependent dielectric factor ($\varepsilon = 4 R_{ij}$) was used.

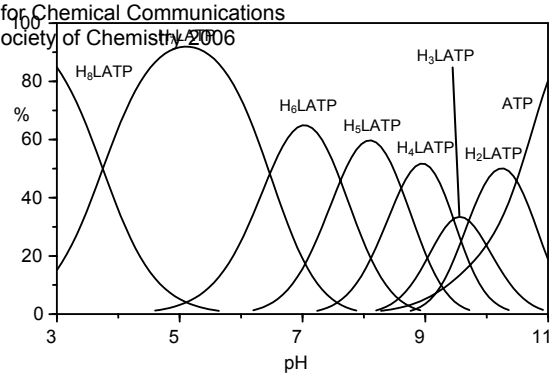


Figure S1. Distribution diagram for the system L-ATP ([L] = [ATP] = $1x10^{-3}$ M, NMe_4Cl 0.1 M, 298.1 K)

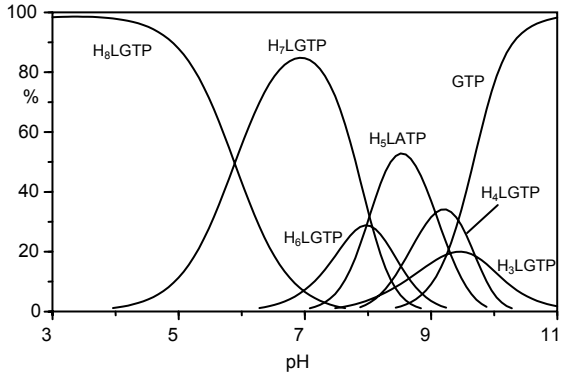


Figure S2. Distribution diagram for the system L-GTP ([L] = [GTP] = $1x10^{-3}$ M, NMe_4Cl 0.1 M, 298.1 K)

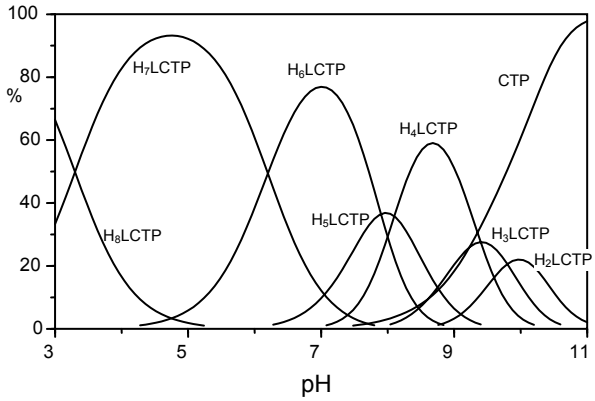


Figure S3. Distribution diagram for the system L-CTP ([L] = [CTP] = $1x10^{-3}$ M, NMe_4Cl 0.1 M, 298.1 K)

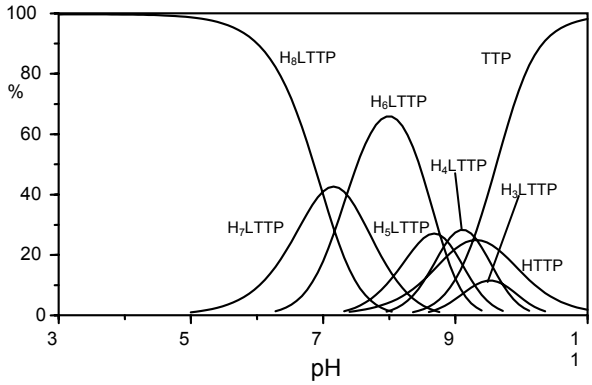


Figure S4. Distribution diagram for the system L-TTP ([L] = [TTP] = $1x10^{-3}$ M, NMe_4Cl 0.1 M, 298.1 K)

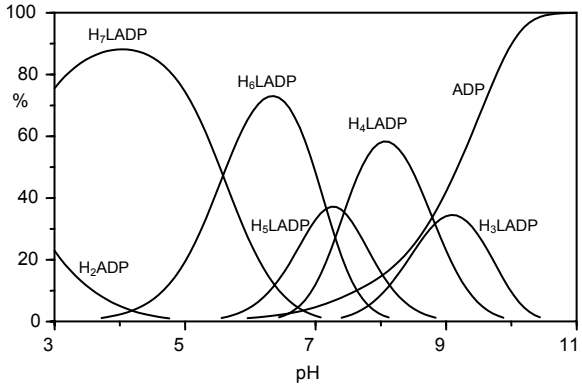


Figure S5. Distribution diagram for the system L-ADP ([L] = [ADP] = $1x10^{-3}$ M, NMe_4Cl 0.1 M, 298.1 K)

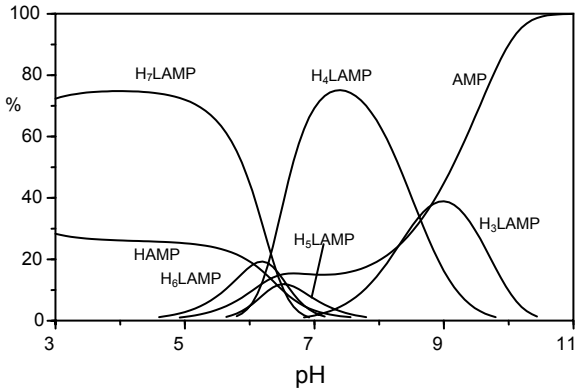


Figure S6. Distribution diagram for the system L-AMP ([L] = [AMP] = $1x10^{-3}$ M, NMe_4Cl 0.1 M, 298.1 K)

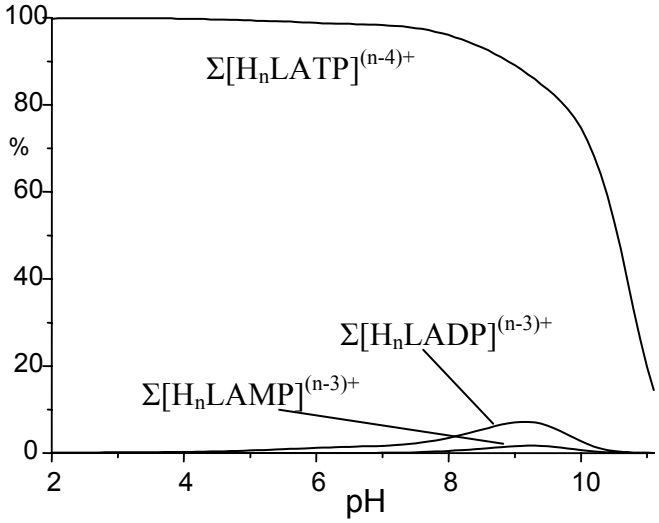


Figure S7. Overall percentages of L complexed species as a function of pH in a competing system containing L, ATP, ADP and AMP in equimolecular ratio at 298 K ([L] = [ATP] = [ADP] = [AMP] = 0.001 M)

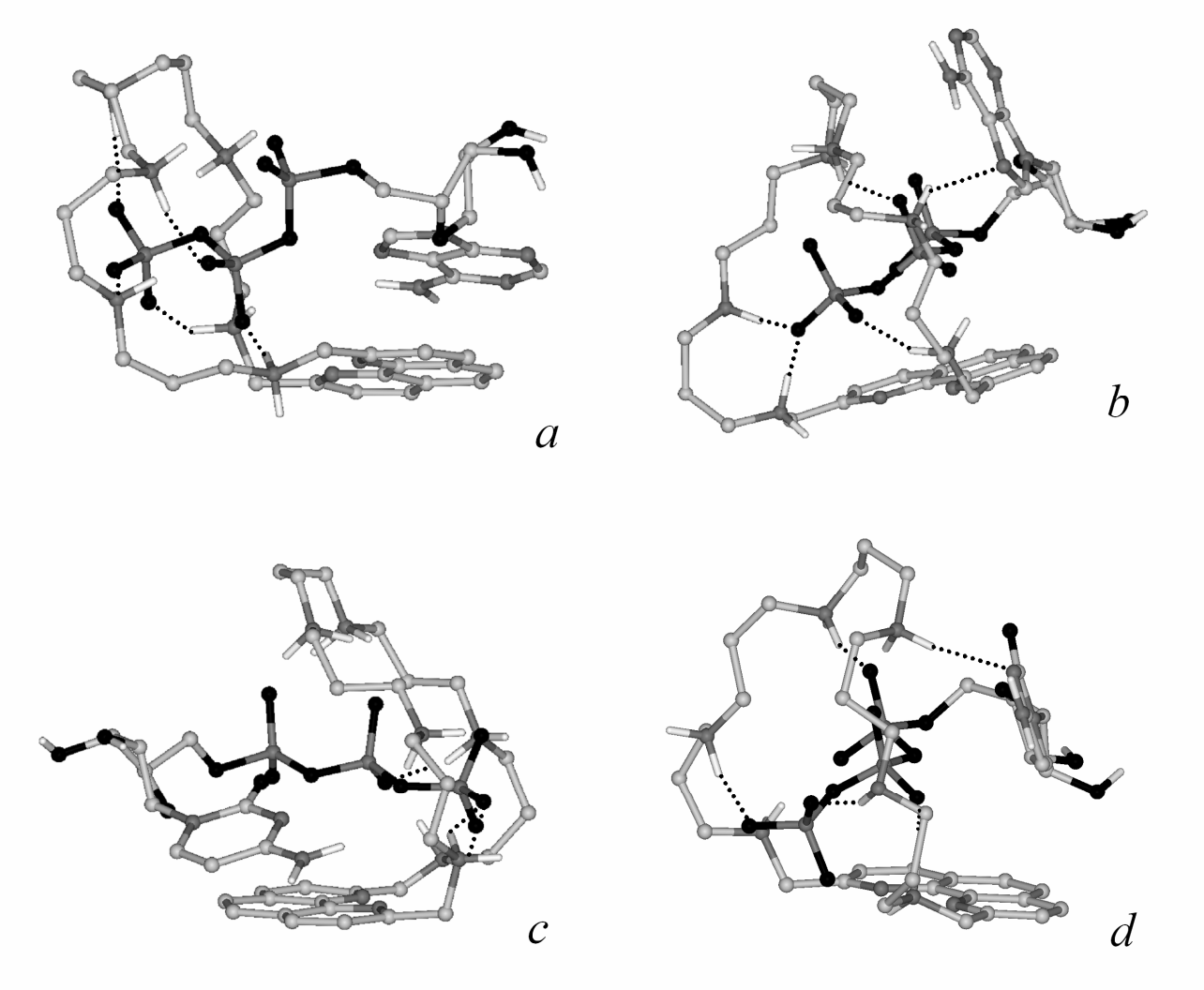


Figure S8. Low energy conformers of the adducts between $[H_6L]^{6+}$ and ATP in the A (a) and B (b) families and between $[H_6L]^{6+}$ and CTP in the A (a) and B (b) families. Only hydrogen bonds with N-H···O distances lower than 2 Å are reported.

Table S1. Protonation constants of L and of nucleotides (0.1 M NMe_4Cl, 298. 1 K)

Reaction	LogK
$L + H^+ = [HL]^+$	10.14 (1)[a]
$[HL]^+ + H^+ = [H_2L]^{2+}$	10.10 (1)
$[H_2L]^{2+} + H^+ = [H_3L]^{3+}$	8.59 (1)
$[H_3L]^{3+} + H^+ = [H_4L]^{4+}$	7.79 (1)
$[H_4L]^{4+} + H^+ = [H_5L]^{5+}$	6.98 (1)
$[H_5L]^{5+} + H^+ = [H_6L]^{6+}$	6.90 (2)

Reaction	Log K	
	ATP	CTP
$A^{4-} + H^+ = HA^{3-}$	6.83(1)	6.23(1)
$HA^{3-} + H^+ = H_2A^{2-}$	4.13(1)	3.81(1)
$H_2A^{2-} + H^+ = H_3A^-$	1.80(2)	
	GTP	TTP
$A^{5-} + H^+ = HA^{4-}$	9.25(1)	9.27(1)
$HA^{4-} + H^+ = H_2A^{3-}$	7.13(1)	6.90(1)
$H_2A^{3-} + H^+ = H_3A^{2-}$	3.24(1)	3.3(1)
	ADP	
$A^{3-} + H^+ = HA^{2-}$	6.49(1)	
$HA^{2-} + H^+ = H_2A^-$	4.98(1)	
	AMP	
$A^{3-} + H^+ = HA^{2-}$	6.24(1)	

Table S2. Cumulative formation constants of the adducts of ATP, TTP, CTP and GTP with L (0.1 M NMe_4Cl, 298. 1 K)

Reaction	Log β	
	A^{4-} = ATP	A^{4-} = CTP
$L + 2\ H^+ + A^{4-} = [H_2LA]^{2-}$	24.53(2)	23.40(3)
$L + 3\ H^+ + A^{4-} = [H_3LA]^{-}$	34.24(2)	33.21(3)
$L + 4\ H^+ + A^{4-} = [H_4LA]$	43.70(2)	42.60(3)
$L + 5\ H^+ + A^{4-} = [H_5LA]^{+}$	52.31(2)	50.69(4)
$L + 6\ H^+ + A^{4-} = [H_6LA]^{2+}$	59.93(3)	58.64(5)
$L + 7\ H^+ + A^{4-} = [H_7LA]^{3+}$	66.40(3)	64.83(5)
$L + 8\ H^+ + A^{4-} = [H_8LA]^{4+}$	70.15(3)	68.10(5)
	A^{5-} = TTP	A^{4-} = GTP
$L + 3\ H^+ + A^{5-} = [H_3LA]^{2-}$	32.54(3)	32.36(1)
$L + 4\ H^+ + A^{5-} = [H_5LA]^{-}$	42.25(3)	42.55(2)
$L + 5\ H^+ + A^{5-} = [H_5LA]$	51.13(4)	51.62(3)
$L + 6\ H^+ + A^{5-} = [H_6LA]^{+}$	59.90(4)	59.60(3)
$L + 7\ H^+ + A^{5-} = [H_7LA]^{2+}$	67.26(4)	67.67(3)
$L + 8\ H^+ + A^{5-} = [H_8LA]^{3+}$	74.25(4)	73.56(6)

Table S3. Stepwise formation constants of the adducts of ATP, TTP, CTP and GTP with L (0.1 M NMe_4Cl, 298. 1 K)

Reaction	Log K	
	$ATP = A^{4-}$	$CTP = A^{4-}$
$[H_2L]^{2+} + A^{4-} = [H_2LA]^{2-}$	4.29	3.16
$[H_3L]^{3+} + A^{4-} = [H_3LA]^{-}$	5.41	4.38
$[H_4L]^{4+} + A^{4-} = [H_4LA]$	7.08	5.98
$[H_4L]^{4+} + [HA]^{3-} = [H_5LA]^{+}$	8.86	7.84
$[H_5L]^{5+} + [A]^{4-} = [H_5LA]^{2+}$	8.89	7.27
$[H_5L]^{5+} + [HA]^{3-} = [H_6LA]^{2+}$	9.68	8.95
$[H_6L]^{6+} + [HA]^{3-} = [H_7LA]^{3+}$	9.55	8.58
$[H_6L]^{6+} + A^{4-} = [H_6LA]^{2+}$	9.91	8.62
$[H_6L]^{6+} + [H_2A]^{2-} = [H_8LA]^{2+}$	9.17	8.06
	$TTP = A^{5-}$	$GTP = A^{5-}$
$[H_2L]^{2+} + [HA]^{4-} = [H_3LA]^{2-}$	3.03	2.87
$[H_3L]^{3+} + [HA]^{4-} = [H_4LA]^{-}$	4.15	4.47
$[H_4L]^{4+} + [HA]^{4-} = [H_5LA]$	5.24	5.75
$[H_4L]^{4+} + [H_2A]^{3-} = [H_6LA]^{+}$	7.11	6.60
$[H_5L]^{5+} + [HA]^{4-} = [H_6LA]^{+}$	7.21	6.93
$[H_5L]^{5+} + [H_2A]^{3-} = [H_7LA]^{2+}$	7.67	7.87
$[H_6L]^{6+} + [HA]^{4-} = [H_7LA]^{2+}$	7.98	8.40
$[H_6L]^{6+} + [H_2A]^{2-} = [H_8LA]^{2+}$	8.06	7.16

Table S4. Cumulative formation constants of the adducts of ADP and AMP with L (0.1 M NMe_4Cl, 298. 1 K)

A = ADP^{3-}

Reaction	Log β
$L + 3\ H^+ + A^{3-} = [H_3LA]$	32.70(2)
$L + 4\ H^+ + A^{3-} = [H_4LA]^+$	41.53(2)
$L + 5\ H^+ + A^{3-} = [H_5LA]^{2+}$	48.97(2)
$L + 6\ H^+ + A^{3-} = [H_6LA]^{3+}$	56.12(2)
$L + 7\ H^+ + A^{3-} = [H_7LA]^{4+}$	61.71(3)

A = AMP^{2-}

Reaction	Log β
$L + 3\ H^+ + A^{2-} = [H_3LA]^+$	32.10(5)
$L + 4\ H^+ + A^{2-} = [H_4LA]^{2+}$	40.72(5)
$L + 5\ H^+ + A^{2-} = [H_5LA]^{3+}$	46.73(7)
$L + 6\ H^+ + A^{2-} = [H_6LA]^{4+}$	53.30(7)
$L + 7\ H^+ + A^{2-} = [H_7LA]^{5+}$	59.67(7)

Table S5. Stepwise formation constants of the adducts of ATP, TTP, CTP and GTP with L (0.1 M NMe_4Cl, 298. 1 K)

$A = ADP^{3-}$

Reaction	Log K
$[H_3L]^{3+} + A^{3-} = [H_3LA]$	3.87
$[H_4L]^{4+} + A^{3-} = [H_4LA]^{-}$	4.91
$[H_4L]^{4+} + [HA]^{2-} = [H_5LA]^{2+}$	5.76
$[H_5L]^{5+} + [A]^{3-} = [H_5LA]^{2+}$	5.55
$[H_5L]^{5+} + [HA]^{2-} = [H_6LA]^{3+}$	6.11
$[H_6L]^{6+} + A^{3-} = [H_6LA]^{3+}$	6.10
$[H_6L]^{6+} + [HA]^{2-} = [H_7LA]^{4+}$	5.10

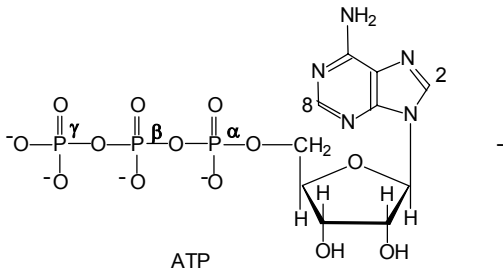
$A = AMP^{2-}$

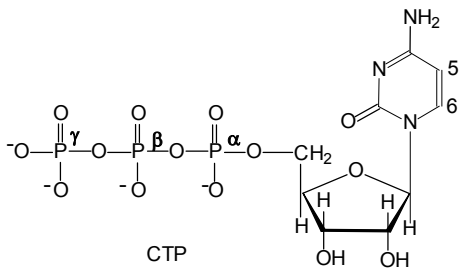
Reaction	Log K
$[H_3L]^{3+} + A^{2-} = [H_3LA]^{-}$	3.27
$[H_4L]^{4+} + A^{2-} = [H_4LA]$	4.25
$[H_4L]^{4+} + [HA]^{-} = [H_5LA]^{+}$	3.87
$[H_5L]^{5+} + [A]^{2-} = [H_6LA]^{2+}$	4.31
$[H_5L]^{5+} + [HA]^{-} = [H_6LA]^{2+}$	3.64
$[H_6L]^{6+} + A^{2-} = [H_6LA]^{2+}$	3.28
$[H_6L]^{6+} + [HA]^{-} = [H_7LA]^{3+}$	3.30

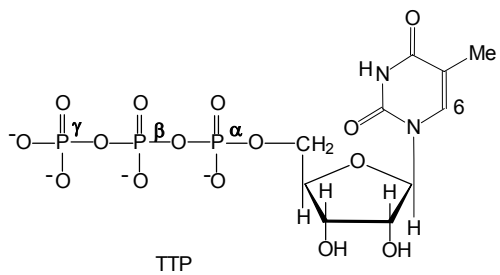
Table S6. ^{31}P NMR shifts (δ, ppm) for the L adducts with ATP, ADP, AMP, CTP, GTP and TTP and complexation-induced ^{31}P NMR chemical shifts (CIS, ppm), measured in D_2O solution at pH 6, 298 K.

	ATP			ADP		AMP
	P_α	P_β	P_γ	P_α	P_β	P_α
δ(ppm)	-9.9	-20.3	-5.2	-8.1	-5.5	-6.1
CIS	1.0	2.7	4.8	0.4	2.1	1.4

	CTP			TTP			GTP		
	P_α	P_β	P_γ	P_α	P_β	P_γ	P_α	P_β	P_γ
δ(ppm)	-10.5	-21.5	-6.5	-10.8	-22.2	-7.6	-10.9	-21.9	-7.4
CIS	0.4	1.2	3.8	0.1	0.9	2.9	0.2	1.1	3.2







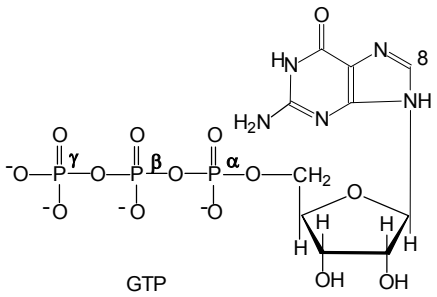


Table S7. ^{1}H NMR shifts (δ, ppm) of the aromatic protons of L and of nucleotides in the complexes with ATP, ADP, AMP, TTP, GTP and CTP and corresponding complexation-induced ^{1}H NMR chemical shifts (CIS, ppm), measured in D_2O solution at pH 6 and 298 K.

		H7	H6	H8	H8	H2
L	δ	8.27	7.63	7.65		
ATP	δ				7.91	7.49
	CIS	-0.26	-0.32	-0.14	-0.60	-0.76

		H8	H2
L	δ	7.72	
ADP	δ		8.21	7.76
	CIS	-0.16	-0.19	-0.08	-0.32	-0.46

		H8	H2
L	δ	8.39	7.80	7.70		
AMP	δ				8.30	7.88
	CIS	-0.14	-0.15	-0.10	-0.21	-0.32

		H6	H5
L	δ[a]	8.39	7.73	7.72		
CTP	δ				7.67	6.02
	CIS	-0.14	-0.22	-0.08	-0.28	-0.20

		H6
L	δ[a]	8.35	7.75	7.71	
TTP	δ				7.43	
	CIS	-0.18	-0.20	-0.09	-0.35	

		H8
L	δ[a]	8.35	7.67	7.70	
GTP	δ				7.79	
	CIS	-0.23	-0.28	-0.10	-0.44	

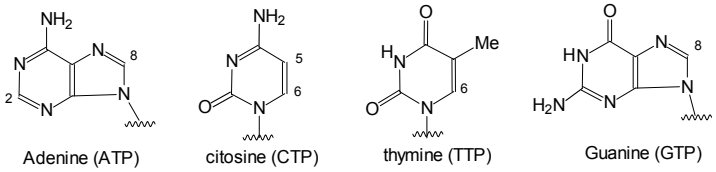


Table S8. Atomic coordinates and atomic charge of the lowest energy conformer of the adducts between $[H_6L]^{6+}$ and ATP in the A family

Atom	Atom type	X	Y	Z	Atomic charge
C1	CA	-1.105	-3.798	-3.485	-0.1328
C2	CA	-0.601	-3.601	-2.186	-0.17513
N3	NC	0.498	-2.846	-1.995	0.01778
C4	CA	1.149	-2.245	-3.009	-0.03796
C5	CA	0.683	-2.396	-4.332	-0.02075
C6	CA	-0.449	-3.197	-4.573	0.015618
C7	CA	1.335	-1.734	-5.389	-0.03675
C8	CA	2.466	-0.94	-5.129	-0.02668
C9	CA	2.97	-0.839	-3.819	-0.02637
C10	CA	2.306	-1.485	-2.755	-0.04049
N11	NC	2.806	-1.409	-1.506	0.009749
C12	CA	3.935	-0.735	-1.211	-0.16911
C13	CA	4.624	-0.051	-2.231	-0.12625
C14	CA	4.139	-0.104	-3.549	0.011956
C15	CT	-1.245	-4.25	-0.979	-0.14554
N16	N3	-1.839	-3.209	-0.121	0.577409
C17	CT	-3.183	-2.755	-0.537	-0.20284
C18	CT	-3.733	-1.677	0.407	-0.11698
C19	CT	-3.074	-0.317	0.143	-0.20093
N20	N3	-3.14	0.599	1.299	0.589054
C21	CT	-4.472	0.805	1.899	-0.20577
C22	CT	-4.583	2.145	2.641	-0.12394
C23	CT	-3.474	2.453	3.661	-0.20394
N24	N3	-3.348	1.425	4.715	0.589252
C25	CT	-2.623	1.874	5.926	-0.2095
C26	CT	-1.169	2.319	5.675	-0.11103
C27	CT	-0.389	1.207	4.968	-0.20351
N28	N3	1.073	1.417	4.869	0.585195
C29	CT	1.854	1.411	6.128	-0.21388
C30	CT	1.825	0.078	6.903	-0.13443
C31	CT	2.864	-0.963	6.455	-0.20519
N32	N3	2.648	-1.47	5.085	0.572408
C33	CT	3.563	-2.575	4.723	-0.19482
C34	CT	3.528	-2.886	3.222	-0.13888
C35	CT	4.308	-1.836	2.415	-0.21261
N36	N3	3.926	-1.854	0.988	0.580888
C37	CT	4.458	-0.715	0.213	-0.1467
H38	HC	-1.981	-4.408	-3.652	0.123905
H39	HC	-0.829	-3.332	-5.575	0.164819
H40	HC	0.959	-1.811	-6.399	0.159174
H41	HC	2.953	-0.428	-5.946	0.159246
H42	HC	5.519	0.511	-2.008	0.134373
H43	HC	4.662	0.416	-4.339	0.166027
H44	HC	-0.462	-4.752	-0.408	0.095495

H45	HC	-1.993	-4.989	-1.268	0.085857
H46	H3	-1.206	-2.421	-0.097	0.108636
H47	H3	-1.907	-3.567	0.823	0.130688
H48	HC	-3.855	-3.613	-0.503	0.1508
H49	HC	-3.155	-2.373	-1.558	0.113028
H50	HC	-3.569	-1.994	1.436	0.047267
H51	HC	-4.809	-1.581	0.248	0.108506
H52	HC	-3.549	0.154	-0.718	0.163462
H53	HC	-2.019	-0.457	-0.084	0.111914
H54	H3	-2.766	1.492	1	0.124064
H55	H3	-2.523	0.246	2.019	0.116603
H56	HC	-4.686	-0.02	2.58	0.091277
H57	HC	-5.224	0.806	1.109	0.122585
H58	HC	-5.548	2.173	3.151	0.123839
H59	HC	-4.575	2.944	1.898	0.084768
H60	HC	-3.729	3.404	4.13	0.084805
H61	HC	-2.521	2.577	3.149	0.146428
H62	H3	-2.896	0.603	4.332	0.1199
H63	H3	-4.28	1.161	5.004	0.137569
H64	HC	-2.617	1.045	6.635	0.15989
H65	HC	-3.168	2.701	6.383	0.120342
H66	HC	-0.725	2.533	6.647	0.044091
H67	HC	-1.143	3.229	5.073	0.097385
H68	HC	-0.755	1.168	3.948	0.160783
H69	HC	-0.606	0.263	5.461	0.12595
H70	H3	1.227	2.298	4.396	0.114203
H71	H3	1.441	0.691	4.265	0.140297
H72	HC	1.475	2.201	6.775	0.11756
H73	HC	2.89	1.656	5.89	0.067235
H74	HC	0.834	-0.372	6.907	0.110313
H75	HC	2.067	0.317	7.94	0.146602
H76	HC	2.808	-1.806	7.145	0.168704
H77	HC	3.861	-0.526	6.523	0.116614
H78	H3	2.784	-0.708	4.435	0.05066
H79	H3	1.692	-1.791	4.986	0.102619
H80	HC	3.255	-3.465	5.273	0.137401
H81	HC	4.587	-2.326	5.007	0.161036
H82	HC	2.486	-2.928	2.901	0.148402
H83	HC	3.979	-3.864	3.044	0.088235
H84	HC	5.378	-2.027	2.507	0.060139
H85	HC	4.107	-0.842	2.811	0.139681
H86	H3	2.917	-1.827	0.928	0.118718
H87	H3	4.245	-2.717	0.572	0.085527
H88	HC	5.548	-0.764	0.207	0.151289
H89	HC	4.146	0.218	0.683	0.104764
P90	P	0.514	1.867	1.101	2.009335
O91	O2	-0.941	2.132	1.185	-1.05022
O92	O2	1.307	2.43	2.22	-0.98477
O93	OS	0.957	2.771	-0.156	-0.67472
C94	CT	2.315	2.912	-0.526	0.159793
H95	HC	2.737	3.792	-0.038	-0.04446
H96	HC	2.89	2.036	-0.224	0.059178

C97	CT	2.431	3.044	-2.047	-0.01126
H98	HC	3.487	3.144	-2.304	0.008287
O99	OS	1.91	1.863	-2.635	-0.18404
C100	CT	0.917	2.21	-3.581	0.080649
H101	HC	1.395	2.318	-4.556	0.033305
N102	N*	-0.151	1.188	-3.627	0.248362
C103	CK	-0.767	0.547	-2.582	-0.29389
H104	HC	-0.488	0.708	-1.555	0.123003
N105	NB	-1.722	-0.266	-2.938	0.032541
C106	CB	-1.744	-0.162	-4.322	-0.19935
C107	CA	-2.528	-0.78	-5.322	-0.01802
N108	N2	-3.5	-1.66	-5.047	0.162375
H109	H2	-3.699	-1.906	-4.088	0.099137
H110	H2	-4.029	-2.082	-5.797	0.001897
N111	NC	-2.272	-0.476	-6.612	-0.3152
C112	CQ	-1.305	0.396	-6.892	-0.02358
H113	HC	-1.147	0.602	-7.94	0.049999
N114	NC	-0.508	1.049	-6.047	-0.27656
C115	CB	-0.781	0.719	-4.754	-0.06355
C116	CT	1.636	4.23	-2.607	0.047367
H117	HC	1.422	4.989	-1.853	0.060904
C118	CT	0.368	3.556	-3.117	0.024474
H119	HC	-0.337	3.419	-2.296	0.133937
O120	OH	-0.236	4.286	-4.164	-0.34059
H121	HO	0.444	4.508	-4.804	0.193113
O122	OH	2.346	4.806	-3.686	-0.33179
O123	O2	0.886	0.501	0.646	-0.88905
P124	P	0.734	-0.564	1.67	2.083591
O125	O2	1.048	-1.861	1.025	-0.98084
O126	O2	1.706	-0.325	2.764	-1.11972
O127	O2	-0.658	-0.577	2.198	-0.89827
P128	P	-1.063	-1.618	3.183	2.036215
O129	O2	-1.314	-2.905	2.498	-1.05457
O130	O2	-0.045	-1.807	4.244	-1.0194
O131	O2	-2.322	-1.145	3.809	-1.03346
H132	HO	2.549	4.118	-4.323	0.159858

Table S9. Atomic coordinates and atomic charge of the lowest energy conformer of the adducts between $[H_6L]^{6+}$ and ATP in the B family

Atom	Atom type	X	Y	Z	Atomic charge
C1	CA	2.162	-1.481	5.784	-0.1328
C2	CA	1.272	-0.444	5.451	-0.17513
N3	NC	1.574	0.404	4.444	0.01778
C4	CA	2.717	0.31	3.731	-0.03796
C5	CA	3.648	-0.708	4.039	-0.02075
C6	CA	3.359	-1.62	5.067	0.015618
C7	CA	4.844	-0.82	3.31	-0.03675
C8	CA	5.123	0.088	2.278	-0.02668
C9	CA	4.191	1.087	1.948	-0.02637
C10	CA	2.988	1.211	2.68	-0.04049
N11	NC	2.121	2.201	2.377	0.009749
C12	CA	2.349	3.083	1.382	-0.16911
C13	CA	3.513	2.976	0.598	-0.12625
C14	CA	4.45	1.976	0.891	0.011956
C15	CT	-0.015	-0.3	6.239	-0.14554
N16	N3	-1.009	0.497	5.495	0.577409
C17	CT	-2.339	0.621	6.13	-0.20284
C18	CT	-3.094	-0.709	6.326	-0.11698
C19	CT	-3.556	-1.408	5.036	-0.20093
N20	N3	-2.456	-2.054	4.289	0.589054
C21	CT	-2.907	-2.816	3.109	-0.20577
C22	CT	-1.717	-3.295	2.268	-0.12394
C23	CT	-2.172	-3.774	0.882	-0.20394
N24	N3	-1.095	-3.608	-0.115	0.589252
C25	CT	-1.277	-4.339	-1.383	-0.2095
C26	CT	-2.464	-3.848	-2.225	-0.11103
C27	CT	-2.25	-2.463	-2.855	-0.20351
N28	N3	-2.702	-1.347	-1.997	0.585195
C29	CT	-2.787	-0.069	-2.733	-0.21388
C30	CT	-3.44	1.039	-1.9	-0.13443
C31	CT	-3.621	2.337	-2.7	-0.20519
N32	N3	-2.359	2.881	-3.25	0.572408
C33	CT	-1.282	3.191	-2.287	-0.19482
C34	CT	-1.721	4.174	-1.191	-0.13888
C35	CT	-0.528	4.735	-0.405	-0.21261
N36	N3	0.282	3.675	0.228	0.580888
C37	CT	1.355	4.188	1.099	-0.1467
H38	HC	1.932	-2.168	6.585	0.123905
H39	HC	4.044	-2.42	5.309	0.164819
H40	HC	5.551	-1.606	3.532	0.159174
H41	HC	6.053	0	1.735	0.159246
H42	HC	3.697	3.661	-0.217	0.134373
H43	HC	5.356	1.899	0.306	0.166027
H44	HC	0.201	0.185	7.192	0.095495
H45	HC	-0.4	-1.3	6.427	0.085857
H46	H3	-1.127	0.095	4.576	0.108636

H47	H3	-0.63	1.425	5.372	0.130688
H48	HC	-2.947	1.282	5.51	0.1508
H49	HC	-2.209	1.094	7.104	0.113028
H50	HC	-4	-0.462	6.882	0.047267
H51	HC	-2.525	-1.401	6.945	0.108506
H52	HC	-4.057	-0.685	4.391	0.163462
H53	HC	-4.274	-2.181	5.313	0.111914
H54	H3	-1.944	-2.67	4.904	0.124064
H55	H3	-1.837	-1.326	3.957	0.116603
H56	HC	-3.526	-2.152	2.505	0.091277
H57	HC	-3.507	-3.672	3.421	0.122585
H58	HC	-1.189	-4.099	2.783	0.123839
H59	HC	-1.019	-2.47	2.147	0.084768
H60	HC	-3.028	-3.189	0.548	0.084805
H61	HC	-2.465	-4.821	0.954	0.146428
H62	H3	-0.228	-3.937	0.291	0.1199
H63	H3	-0.974	-2.623	-0.317	0.137569
H64	HC	-1.412	-5.397	-1.159	0.15989
H65	HC	-0.361	-4.235	-1.967	0.120342
H66	HC	-3.393	-3.874	-1.657	0.044091
H67	HC	-2.563	-4.557	-3.05	0.097385
H68	HC	-2.83	-2.44	-3.778	0.160783
H69	HC	-1.2	-2.321	-3.105	0.12595
H70	H3	-2.064	-1.237	-1.216	0.114203
H71	H3	-3.619	-1.568	-1.638	0.140297
H72	HC	-3.377	-0.212	-3.638	0.11756
H73	HC	-1.776	0.227	-3.003	0.067235
H74	HC	-2.837	1.24	-1.02	0.110313
H75	HC	-4.422	0.701	-1.566	0.146602
H76	HC	-4.093	3.085	-2.062	0.168704
H77	HC	-4.294	2.142	-3.536	0.116614
H78	H3	-2.583	3.73	-3.748	0.05066
H79	H3	-1.993	2.215	-3.916	0.102619
H80	HC	-0.458	3.629	-2.85	0.137401
H81	HC	-0.932	2.265	-1.836	0.161036
H82	HC	-2.396	3.676	-0.494	0.148402
H83	HC	-2.246	5.013	-1.65	0.088235
H84	HC	-0.911	5.397	0.372	0.060139
H85	HC	0.106	5.315	-1.077	0.139681
H86	H3	0.695	3.097	-0.493	0.118718
H87	H3	-0.323	3.084	0.782	0.085527
H88	HC	0.922	4.55	2.032	0.151289
H89	HC	1.867	5.015	0.605	0.104764
P90	P	2.134	-2.2	0.724	2.009335
O91	O2	1.818	-2.284	2.168	-1.05022
O92	O2	1.569	-3.307	-0.082	-0.98477
O93	OS	3.721	-2.509	0.693	-0.67472
C94	CT	4.372	-3.091	-0.429	0.159793
H95	HC	5.396	-3.3	-0.12	-0.04446
H96	HC	3.905	-4.041	-0.689	0.059178
C97	CT	4.449	-2.197	-1.678	-0.01126
H98	HC	5.075	-2.716	-2.406	0.008287

O99	OS	3.202	-1.984	-2.314	-0.18404
C100	CT	3.375	-0.83	-3.113	0.080649
H101	HC	4.023	-1.081	-3.954	0.033305
N102	N*	2.093	-0.304	-3.64	0.248362
C103	CK	1.61	0.983	-3.638	-0.29389
H104	HC	2.1	1.801	-3.13	0.123003
N105	NB	0.511	1.146	-4.318	0.032541
C106	CB	0.236	-0.122	-4.815	-0.19935
C107	CA	-0.79	-0.634	-5.642	-0.01802
N108	N2	-1.775	0.126	-6.141	0.162375
H109	H2	-1.8	1.114	-5.937	0.099137
H110	H2	-2.483	-0.287	-6.731	0.001897
N111	NC	-0.764	-1.947	-5.953	-0.3152
C112	CQ	0.225	-2.705	-5.48	-0.02358
H113	HC	0.196	-3.747	-5.764	0.049999
N114	NC	1.245	-2.344	-4.704	-0.27656
C115	CB	1.192	-1.017	-4.397	-0.06355
C116	CT	5.05	-0.808	-1.425	0.047367
H117	HC	5.057	-0.561	-0.368	0.060904
C118	CT	4.11	0.133	-2.181	0.024474
H119	HC	3.408	0.584	-1.481	0.133937
O120	OH	4.811	1.14	-2.881	-0.34059
H121	HO	5.547	0.726	-3.338	0.193113
O122	OH	6.364	-0.746	-1.944	-0.33179
O123	O2	2.062	-0.843	0.124	-0.88905
P124	P	0.694	-0.272	0.005	2.083591
O125	O2	0.823	1.082	-0.584	-0.98084
O126	O2	-0.124	-1.108	-0.911	-1.11972
O127	O2	0.063	-0.184	1.353	-0.89827
P128	P	-1.34	0.297	1.468	2.036215
O129	O2	-1.461	1.702	1.019	-1.05457
O130	O2	-2.263	-0.559	0.684	-1.0194
O131	O2	-1.74	0.222	2.891	-1.03346
H132	HO	6.904	-1.392	-1.483	0.159858

Table S10. Atomic coordinates and atomic charge of the lowest energy conformer of the adducts between $[H_6L]^{6+}$ and CTP in the A family

Atom	Atom type	X	Y	Z	Atomic charge
C1	CA	-0.103	-4.153	1.937	-0.1328
C2	CA	-1.22	-3.367	2.277	-0.17513
N3	NC	-1.839	-2.631	1.333	0.01778
C4	CA	-1.443	-2.628	0.043	-0.03796
C5	CA	-0.356	-3.435	-0.359	-0.02075
C6	CA	0.337	-4.186	0.605	0.015618
C7	CA	0.002	-3.516	-1.716	-0.03675
C8	CA	-0.775	-2.863	-2.686	-0.02668
C9	CA	-1.855	-2.054	-2.292	-0.02637
C10	CA	-2.151	-1.884	-0.921	-0.04049
N11	NC	-3.128	-1.031	-0.55	0.009749
C12	CA	-3.875	-0.355	-1.445	-0.16911
C13	CA	-3.689	-0.569	-2.824	-0.12625
C14	CA	-2.659	-1.42	-3.253	0.011956
C15	CT	-1.754	-3.377	3.694	-0.14554
N16	N3	-1.636	-2.035	4.291	0.577409
C17	CT	-1.998	-2.006	5.723	-0.20284
C18	CT	-1.971	-0.598	6.337	-0.11698
C19	CT	-0.566	0.014	6.453	-0.20093
N20	N3	-0.166	0.732	5.227	0.589054
C21	CT	1.164	1.37	5.274	-0.20577
C22	CT	2.308	0.348	5.183	-0.12394
C23	CT	3.637	1.035	4.849	-0.20394
N24	N3	3.757	1.394	3.417	0.589252
C25	CT	4.934	2.255	3.173	-0.2095
C26	CT	5.336	2.366	1.696	-0.11103
C27	CT	4.453	3.274	0.828	-0.20351
N28	N3	3.135	2.696	0.489	0.585195
C29	CT	2.519	3.393	-0.662	-0.21388
C30	CT	1.054	3.009	-0.9	-0.13443
C31	CT	0.083	3.788	0	-0.20519
N32	N3	-1.336	3.511	-0.32	0.572408
C33	CT	-1.806	4.084	-1.6	-0.19482
C34	CT	-3.335	4.061	-1.752	-0.13888
C35	CT	-3.92	2.665	-2.009	-0.21261
N36	N3	-4.307	1.968	-0.765	0.580888
C37	CT	-4.911	0.634	-0.952	-0.1467
H38	HC	0.422	-4.726	2.687	0.123905
H39	HC	1.198	-4.779	0.336	0.164819
H40	HC	0.845	-4.116	-2.027	0.159174
H41	HC	-0.526	-2.974	-3.731	0.159246
H42	HC	-4.299	-0.054	-3.552	0.134373
H43	HC	-2.48	-1.562	-4.309	0.166027
H44	HC	-1.191	-4.091	4.297	0.095495
H45	HC	-2.802	-3.678	3.679	0.085857
H46	H3	-2.239	-1.399	3.784	0.108636

H47	H3	-0.684	-1.714	4.171	0.130688
H48	HC	-1.326	-2.658	6.282	0.1508
H49	HC	-3.014	-2.392	5.822	0.113028
H50	HC	-2.368	-0.69	7.349	0.047267
H51	HC	-2.63	0.07	5.78	0.108506
H52	HC	0.157	-0.764	6.696	0.163462
H53	HC	-0.581	0.739	7.267	0.111914
H54	H3	-0.85	1.454	5.038	0.124064
H55	H3	-0.179	0.09	4.446	0.116603
H56	HC	1.261	1.958	6.188	0.091277
H57	HC	1.22	2.057	4.432	0.122585
H58	HC	2.106	-0.409	4.425	0.123839
H59	HC	2.408	-0.15	6.148	0.084768
H60	HC	4.449	0.349	5.095	0.084805
H61	HC	3.736	1.927	5.468	0.146428
H62	H3	2.919	1.871	3.111	0.1199
H63	H3	3.844	0.548	2.866	0.137569
H64	HC	5.784	1.813	3.695	0.15989
H65	HC	4.757	3.249	3.586	0.120342
H66	HC	5.423	1.376	1.249	0.044091
H67	HC	6.333	2.809	1.683	0.097385
H68	HC	4.998	3.434	-0.104	0.160783
H69	HC	4.317	4.24	1.314	0.12595
H70	H3	2.521	2.753	1.291	0.114203
H71	H3	3.25	1.716	0.262	0.140297
H72	HC	3.088	3.121	-1.552	0.11756
H73	HC	2.587	4.473	-0.526	0.067235
H74	HC	0.927	1.94	-0.739	0.110313
H75	HC	0.831	3.232	-1.944	0.146602
H76	HC	0.265	4.859	-0.096	0.168704
H77	HC	0.259	3.511	1.038	0.116614
H78	H3	-1.895	3.915	0.418	0.05066
H79	H3	-1.489	2.512	-0.317	0.102619
H80	HC	-1.354	3.555	-2.439	0.137401
H81	HC	-1.493	5.128	-1.643	0.161036
H82	HC	-3.57	4.672	-2.625	0.148402
H83	HC	-3.811	4.522	-0.884	0.088235
H84	HC	-3.195	2.076	-2.567	0.060139
H85	HC	-4.818	2.777	-2.618	0.139681
H86	H3	-4.977	2.547	-0.28	0.118718
H87	H3	-3.494	1.87	-0.172	0.085527
H88	HC	-5.75	0.693	-1.646	0.151289
H89	HC	-5.287	0.293	0.014	0.104764
P90	P	2.332	-1.041	0.792	2.087527
O91	O2	3.412	-0.05	1.023	-1.08131
O92	O2	2.386	-2.223	1.681	-1.07089
O93	OS	2.72	-1.662	-0.645	-0.63096
C94	CT	3.338	-0.872	-1.644	0.142772
H95	HC	2.843	0.096	-1.728	-0.0179
H96	HC	4.379	-0.713	-1.364	0.050401
C97	CT	3.279	-1.597	-2.993	-0.01572
H98	HC	3.677	-2.606	-2.874	0.038706

O99	OS	1.929	-1.642	-3.437	-0.26788
C100	CT	1.821	-0.955	-4.673	0.095785
H101	HC	1.978	-1.702	-5.454	0.047496
N102	N*	0.515	-0.27	-4.889	0.088225
C103	CM	-0.119	-0.371	-6.106	-0.16253
H104	HC	0.301	-1.007	-6.872	0.18304
C105	CM	-1.251	0.321	-6.38	-0.26524
H106	HC	-1.719	0.218	-7.349	0.134639
C107	CA	-1.762	1.176	-5.342	-0.02526
N108	N2	-2.874	1.894	-5.549	0.073909
H109	H2	-3.355	1.837	-6.436	0.038961
H110	H2	-3.233	2.492	-4.818	0.023416
N111	NC	-1.143	1.265	-4.153	-0.40809
C112	C	-0.011	0.552	-3.885	0.292746
O113	O	0.524	0.638	-2.784	-0.53392
C114	CT	4.075	-0.832	-4.057	0.033716
H115	HC	4.879	-0.224	-3.639	0.166244
C116	CT	2.995	0.021	-4.706	0.025158
H117	HC	2.797	0.899	-4.091	0.070469
O118	OH	3.346	0.406	-6.019	-0.38432
H119	HO	2.608	0.885	-6.404	0.221
O120	OH	4.599	-1.738	-5.006	-0.38209
O121	O2	0.983	-0.475	0.533	-0.90619
P122	P	0.385	0.266	1.674	2.100363
O123	O2	0.221	-0.636	2.841	-1.03725
O124	O2	1.272	1.397	2.055	-1.11025
O125	O2	-0.934	0.799	1.232	-0.8869
P126	P	-1.851	1.364	2.261	2.042111
O127	O2	-2.437	0.286	3.088	-1.07525
O128	O2	-1.151	2.327	3.141	-0.95794
O129	O2	-2.94	2.081	1.562	-1.03394
H130	HO	4.818	-1.241	-5.799	0.297155

Table S10. Atomic coordinates and atomic charge of the lowest energy conformer of the adducts between $[H_6L]^{6+}$ and CTP in the B family

Atom	Atom type	X	Y	Z	Atomic charge
C1	CA	-3.668	1.422	-1.725	-0.1328
C2	CA	-2.397	1.988	-1.509	-0.17513
N3	NC	-1.325	1.498	-2.163	0.01778
C4	CA	-1.405	0.463	-3.02	-0.03796
C5	CA	-2.655	-0.142	-3.275	-0.02075
C6	CA	-3.8	0.35	-2.623	0.015618
C7	CA	-2.742	-1.233	-4.159	-0.03675
C8	CA	-1.585	-1.719	-4.792	-0.02668
C9	CA	-0.339	-1.109	-4.55	-0.02637
C10	CA	-0.249	-0.009	-3.67	-0.04049
N11	NC	0.934	0.612	-3.487	0.009749
C12	CA	2.059	0.222	-4.115	-0.16911
C13	CA	2.033	-0.887	-4.983	-0.12625
C14	CA	0.823	-1.568	-5.194	0.011956
C15	CT	-2.23	3.16	-0.563	-0.14554
N16	N3	-0.83	3.224	-0.097	0.577409
C17	CT	-0.481	4.387	0.745	-0.20284
C18	CT	-1.214	4.41	2.093	-0.11698
C19	CT	-1.092	3.099	2.88	-0.20093
N20	N3	0.306	2.748	3.202	0.589054
C21	CT	0.404	1.495	3.972	-0.20577
C22	CT	1.853	1.143	4.32	-0.12394
C23	CT	1.933	-0.141	5.151	-0.20394
N24	N3	1.259	-1.284	4.496	0.589252
C25	CT	1.447	-2.565	5.208	-0.2095
C26	CT	2.824	-3.208	4.989	-0.11103
C27	CT	3.073	-3.637	3.532	-0.20351
N28	N3	3.641	-2.576	2.673	0.585195
C29	CT	4.969	-2.072	3.089	-0.21388
C30	CT	5.788	-1.532	1.909	-0.13443
C31	CT	5.053	-0.402	1.178	-0.20519
N32	N3	5.819	0.171	0.053	0.572408
C33	CT	6.168	-0.799	-1.006	-0.19482
C34	CT	6.646	-0.122	-2.298	-0.13888
C35	CT	5.613	0.814	-2.943	-0.21261
N36	N3	4.314	0.152	-3.183	0.580888
C37	CT	3.342	0.996	-3.898	-0.1467
H38	HC	-4.536	1.807	-1.211	0.123905
H39	HC	-4.769	-0.097	-2.79	0.164819
H40	HC	-3.692	-1.713	-4.346	0.159174
H41	HC	-1.661	-2.561	-5.466	0.159246
H42	HC	2.929	-1.212	-5.49	0.134373
H43	HC	0.79	-2.414	-5.865	0.166027
H44	HC	-2.898	3.034	0.288	0.095495
H45	HC	-2.483	4.079	-1.092	0.085857
H46	H3	-0.228	3.248	-0.91	0.108636

H47	H3	-0.614	2.369	0.4	0.130688
H48	HC	-0.708	5.303	0.198	0.1508
H49	HC	0.594	4.366	0.924	0.113028
H50	HC	-2.272	4.613	1.922	0.047267
H51	HC	-0.81	5.226	2.694	0.108506
H52	HC	-1.535	2.286	2.308	0.163462
H53	HC	-1.651	3.208	3.81	0.111914
H54	H3	0.72	3.497	3.737	0.124064
H55	H3	0.828	2.634	2.343	0.116603
H56	HC	-0.025	0.704	3.359	0.091277
H57	HC	-0.167	1.595	4.895	0.122585
H58	HC	2.297	1.96	4.891	0.123839
H59	HC	2.434	1.008	3.409	0.084768
H60	HC	1.465	0.034	6.121	0.084805
H61	HC	2.986	-0.369	5.311	0.146428
H62	H3	1.575	-1.365	3.537	0.1199
H63	H3	0.267	-1.088	4.475	0.137569
H64	HC	0.692	-3.274	4.874	0.15989
H65	HC	1.291	-2.405	6.276	0.120342
H66	HC	2.833	-4.118	5.592	0.044091
H67	HC	3.624	-2.57	5.362	0.097385
H68	HC	2.141	-3.986	3.083	0.160783
H69	HC	3.773	-4.473	3.533	0.12595
H70	H3	2.993	-1.803	2.598	0.114203
H71	H3	3.725	-2.974	1.745	0.140297
H72	HC	5.542	-2.885	3.536	0.11756
H73	HC	4.843	-1.284	3.832	0.067235
H74	HC	5.974	-2.359	1.223	0.110313
H75	HC	6.744	-1.161	2.282	0.146602
H76	HC	4.815	0.401	1.877	0.168704
H77	HC	4.128	-0.801	0.775	0.116614
H78	H3	6.667	0.592	0.405	0.05066
H79	H3	5.245	0.899	-0.353	0.102619
H80	HC	5.309	-1.431	-1.227	0.137401
H81	HC	6.974	-1.439	-0.646	0.161036
H82	HC	6.901	-0.903	-3.016	0.148402
H83	HC	7.55	0.451	-2.085	0.088235
H84	HC	6.017	1.147	-3.9	0.060139
H85	HC	5.468	1.695	-2.319	0.139681
H86	H3	3.903	-0.135	-2.303	0.118718
H87	H3	4.477	-0.678	-3.735	0.085527
H88	HC	3.749	1.294	-4.865	0.151289
H89	HC	3.137	1.892	-3.31	0.104764
P90	P	1.934	-2.336	-0.849	2.087527
O91	O2	2.885	-1.781	-1.841	-1.08131
O92	O2	2.584	-3.078	0.258	-1.07089
O93	OS	1.222	-3.508	-1.703	-0.63096
C94	CT	0.478	-4.561	-1.109	0.142772
H95	HC	0.316	-5.303	-1.892	-0.0179
H96	HC	1.045	-5.039	-0.309	0.050401
C97	CT	-0.905	-4.143	-0.594	-0.01572
H98	HC	-1.466	-5.053	-0.374	0.038706

O99	OS	-0.862	-3.399	0.605	-0.26788
C100	CT	-2.148	-2.824	0.749	0.095785
H101	HC	-2.854	-3.624	0.98	0.047496
N102	N*	-2.233	-1.802	1.838	0.088225
C103	CM	-2.977	-0.649	1.693	-0.16253
H104	HC	-3.43	-0.404	0.747	0.18304
C105	CM	-3.192	0.198	2.728	-0.26524
H106	HC	-3.793	1.083	2.574	0.134639
C107	CA	-2.606	-0.15	3.993	-0.02526
N108	N2	-2.794	0.64	5.06	0.073909
H109	H2	-3.34	1.485	4.973	0.038961
H110	H2	-2.39	0.389	5.951	0.023416
N111	NC	-1.889	-1.276	4.136	-0.40809
C112	C	-1.698	-2.132	3.089	0.292746
O113	O	-1.109	-3.195	3.269	-0.53392
C114	CT	-1.71	-3.289	-1.576	0.033716
H115	HC	-1.057	-2.736	-2.249	0.166244
C116	CT	-2.44	-2.301	-0.662	0.025158
H117	HC	-1.99	-1.317	-0.79	0.070469
O118	OH	-3.826	-2.271	-0.939	-0.38432
H119	HO	-4.127	-3.177	-1.044	0.221
O120	OH	-2.604	-4.098	-2.315	-0.38209
O121	O2	0.805	-1.444	-0.47	-0.90619
P122	P	1.201	-0.262	0.343	2.100363
O123	O2	0.01	0.608	0.515	-1.03725
O124	O2	1.658	-0.706	1.69	-1.11025
O125	O2	2.305	0.466	-0.348	-0.8869
P126	P	2.525	1.916	-0.125	2.042111
O127	O2	3.941	2.213	-0.437	-1.07525
O128	O2	1.657	2.7	-1.031	-0.95794
O129	O2	2.258	2.309	1.278	-1.03394
H130	HO	-2.092	-4.74	-2.812	0.297155